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THESIS

NUMERICAL MODELING OF BLOCH OSCILLATIONS
IN PERIODIC STRUCTURES

by

Walter A. Coppeans III

December, 1996

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Felix Bloch's 1928 article made a prediction concerning the dynamical behavior of electrons in a solid, subject to a uniform, static electric field. This aspect of his work, as later clarified by Zener, showed that electrons accelerated by an electric field in a periodic potential, under the right conditions, would oscillate. A theoretical debate as to the existence of this phenomenon has been ongoing since Bloch's proposal. One of the most controversial consequences of this prediction is that an electron undergoing Bloch oscillations would radiate. The controversy on the theoretical analysis was due to the great difficulty in systematically and reliably treating interband transitions by analytical methods based on the time-dependent Schrodinger equation for independent electrons. In this thesis, we numerically solve the time-dependent Schrodinger equation to show that electrons accelerated by in an electric field in periodic structures do undergo Bloch oscillations and other dynamic behavior. By accurately modeling this phenomenon, we hope to gain a better understanding of it in hopes of using it in future applications as a stable source of Terahertz (THz) radiation.

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NUMERICAL MODELING OF BLOCH OSCILLATIONS IN PERIODIC STRUCTURES

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Submitted in partial fulfillment of the
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ABSTRACT

Felix Bloch's 1928 article made a prediction concerning the dynamical behavior of electrons in a solid, subject to a uniform, static electric field. This aspect of his work, as later clarified by Zener, showed that electrons accelerated by an electric field in a periodic potential, under the right conditions, would oscillate. A theoretical debate as to the existence of this phenomenon has been ongoing since Bloch's proposal. One of the most controversial consequences of this prediction is that an electron undergoing Bloch oscillations would radiate. The controversy on the theoretical analysis was due to the great difficulty in systematically and reliably treating interband transitions by analytical methods based on the time-dependent Schrodinger equation for independent electrons. In this thesis, we numerically solve the time-dependent Schrodinger equation to show that electrons accelerated by in an electric field in periodic structures do undergo Bloch oscillations and other dynamic behavior. By accurately modeling this phenomenon, we hope to gain a better understanding of it in hopes of using it in future applications as a stable source of Terahertz (THz) radiation.

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I. INTRODUCTION

In 1928, Felix Bloch [Ref. 1] wrote a groundbreaking work discussing the quantum mechanical nature of electrons in solids. In this seminal work, Bloch demonstrated what is widely known as "Bloch's theorem," which establishes the mathematical form of the electron wave function of a crystalline solid. We will discuss Bloch's theorem later in this thesis. Bloch's theorem is the basis for our understanding of the all-important energy bands in solids. In addition to establishing Bloch's theorem, a less well known result from Bloch's 1928 article is a prediction concerning the dynamical behavior of electrons in a solid, subject to a uniform, static electric field. This aspect of his work, as later expanded by Zener [Ref. 2], showed that electrons accelerated by an electric field in a periodic potential, under the right conditions would oscillate. The frequency of oscillation is given by the formula $\omega_{_B} = eFa/\hbar$, where e is the charge of an electron, F is the electric field amplitude, a is the lattice repeat distance, and $\hbar$ is Planck's constant h divided by 2π. This phenomenon has come to be known as Bloch oscillations. A theoretical debate as to the existence of this phenomenon has been ongoing since Bloch's proposal. One of the most controversial consequences of this prediction is that an electron undergoing Bloch oscillations would radiate. The controversy on the theoretical analysis was due to the great difficulty in systematically and reliably treating interband transitions by analytical methods based on the time-dependent Schrodinger equation for independent electrons.

With the advent and refinement of semiconductor technology, it has been finally possible to test the predictions of Bloch's proposal. In 1970, Esaki and Tsu [Ref. 3] proposed using a semiconductor superlattice, which would provide the needed periodic structure on a large enough scale in order to conduct tests to generate and detect Bloch oscillations. According to Esaki and Tsu [Ref. 3], the oscillating electron in a semiconductor superlattice would provide a source of Terahertz (THz) radiation. It was only in 1992, however, that Bloch oscillations and the associated Terahertz radiation were conclusively detected in semiconductor superlattices [Ref. 4]. These recent four wave

mixing experiments confirm the presence of photons emitted as a result of the oscillating electron, but noted the oscillations died between 1 and 15 oscillations [Ref. 4]. More recently, Luban and co-workers[Ref. 5] modeled the effect of an electron in a semiconductor superlattice using computer techniques, and showed Bloch oscillations exist at Terahertz frequencies, but did not show the decay as seen in real world experiments. The advantage of a purely numerical approach to solving the time-dependent Schrodinger equation is that one explicitly works with the full Hamiltonian, and not some approximation as in analytical solutions, thus including all interband transitions in the simulation.

This paper will cover the theoretical debates and arguments surrounding the issue. Also, it will develop the theory behind Bloch oscillations. Lastly, it will cover the numerical techniques involved in solving the Time Dependent Schrodinger Equation, and present the results of the simulations.

II. THEORETICAL WORK

In this chapter, we summarize and discuss the works of major contributors on the subject of Bloch oscillations.

A. FELIX BLOCH

In 1928, Felix Bloch wrote a ground breaking paper [Ref. 1] which until recently was the subject of great debate. In it, he used quantum mechanics to model the effects of electrons in periodic (atomic) structures. In this landmark paper, he proved what is now known as Bloch's theorem, which shows that the mathematical form of the eigenvector of the time independent Schrodinger equation must be:

$$\psi_{n,k}(x) = e^{ikx} u_{n,k}(x) \qquad (2.1)$$

where

$$u_{n,k}(x) = u_{n,k}(x + a) \qquad (2.2)$$

and n labels the energy bands and is known as the band index. Also, the parameter k is the allowed wavevector of the electron and is restricted to the Brillouin zone associated with the particular lattice structure of the crystal. The associated energy eigenvalue $E_n(k)$ is called the band structure function.

Bloch showed [Ref. 1] that the wave function of any particle in a periodic potential can be represented as a sum of orthogonal functions that have the periodicity of the lattice structure. Bloch [Ref. 1], starting with the time dependent Schrodinger equation with an external electric field applied:

$$\nabla^2 \psi(x,t) - \frac{2m}{\hbar^2}(V(x) - eFx)\psi(x,t) + \frac{i2m}{\hbar}\frac{\partial \psi(x,t)}{\partial t} = 0 \ , \qquad (2.3)$$

and assuming the following form of the wave function:

$$\psi(x,t) = \sum_{n,k} c_{n,k}(t)\psi_{n,k} e^{-\frac{2\pi i}{h} E_n t} ,$$ (2.4)

derived the result for the time variation of the amplitude of the coefficients of the Bloch functions of the electron wave function:

$$\frac{d}{dt}|c_{n,k}|^2 = -\frac{2\pi eF}{h}\frac{\partial}{\partial k}|c_{n,k}(0)|^2.$$ (2.5)

He also showed for a collection of electrons obeying Fermi statistics [Ref. 1], that the time variation of the electron distribution function $f(k,t)$ is:

$$\frac{df}{dt} = -\frac{2\pi eF}{h}\frac{\partial f}{\partial k}.$$ (2.6)

In (2.6), $f(k,t)$ is the probability of finding an electron between states k and $k + \Delta k$ at time t . Bloch claims this is the same result obtained by Lorentz [Ref. 6] in an earlier paper published in 1916.

B. CLARENCE ZENER

Zener [Ref. 2], in 1933, substantially clarified Bloch's work [Ref. 1] in a paper investigating the breakdown of solids by an electric field. The breakdown of a dielectric under the influence of an electric field takes place by one of two mechanisms [Ref. 2]:

1. A process similar to the electrical breakdown of a gas, i.e., avalanche breakdown.

2. A process like the auto ionization of free atoms in an electric field.

For solids, Zener [Ref . 2] said the second process is more important in a solid than in a gas since the mean free path of an electron is much less for a solid than a gas. An

electron, therefore, tends to become excited and move about in the lattice instead of being freed from the solid completely. He used the Bloch model of an electron to calculate the rate at which electrons move from lower to upper energy bands in a solid under the influence of a constant electric field.

Zener [Ref. 2] started with the same initial wavefunction (2.1). He said that the condition that ψ_k be finite over the lattice imposes the restriction that k be real as well. This only occurs when the electron energy E_n lies within the allowed energy bands that are a solution of the time independent Schrodinger equation, with the first energy band occuring within the values $-\pi/a \leq k \leq \pi/a$ [Ref. 2] for a one dimensional model. Following Bloch, Zener [Ref. 2] expanded his wave function in terms of wave functions of the lowest energy band with no electric field applied:

$$\psi(x,t) = \int_{-\pi/a}^{\pi/a} g(k,t)\psi_{n,k}(x)dk .$$
(2.7)

Following Bloch's derivation, Zener [Ref. 2] reproduced equation (2.5) in a more concise form:

$$\frac{d}{dt}|g|^2 = -\frac{2\pi eF}{h}\frac{\partial}{\partial k}|g|^2$$
(2.8)

where

$$|g|^2 = G\left(k - \frac{2\pi eF}{h}t\right),$$
(2.9)

with G being an arbitrary function. Zener [Ref. 2] also showed that the velocity in k space is $2\pi eF/h$. Using the limits of k, Zener showed the period of time for real space oscillation is:

$$\tau_B = (2\pi/a)/(2\pi eF/h) = \frac{h}{eFa}$$
(2.10)

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or the frequency of oscillation is given by:

$$v_B = \frac{eFa}{h}.$$

(2.11)

Zener [Ref. 2] said than an electron confined to a single energy band will move opposite to the direction of the field until reflected by the lattice, and then it moves in the opposite direction until it is stopped by the field, where it starts the same motion over again. Zener [Ref. 2] then calculated the probability that an electron would undergo transitions between energy bands. Starting with a wave function that is periodic in time, Zener showed the wave equation for an electron when an external field F is present is (2.3). Zener [Ref. 2] found an approximate solution, assuming the term eFx varies slightly over the lattice distance a :

$$\psi_{n,k}(x) = e^{i\int Kdx} u_{n,k}(x)$$

(2.12)

where K is a function of $(E - eFx)$. Using (2.12), and solving for K, Zener [Ref. 2] showed the rate of transition (γ) between energy bands is given by:

$$\gamma = \frac{eFa}{h} \exp\left(-\frac{\pi^2}{h^2} \frac{maE_g^2}{|eF|}\right)$$

(2.13)

where E_g is the energy gap between bands.

C. W. V. HOUSTON

In 1939, Houston [Ref. 7] showed that the wave vector of an electron accelerated by an electric field in a periodic potential grows linearly with time within the bounds of the first Brillouin zone[Ref. 7].

Houston assumed the form of this wave function as:

$$\psi(x,t) = u_{k+\lambda t}(x)e^{i(k+\lambda t)x}e^{-\frac{i}{\hbar}\int^{t}E_{k+\lambda t}d\tau} \tag{2.14}$$

where $\lambda = eF/\hbar$ [Ref. 7], which shows the solution of the time dependent Schrodinger equation is constructed from the solution of the time independent Schrodinger equation, modulated by a time dependent wave vector. Equation (2.14) is a solution of (2.3), with the following remainder:

$$-\left(\frac{\hbar}{i}\right)(\lambda \nabla u_{k+\lambda t})e^{i(k+\lambda t)x}e^{-\frac{i}{\hbar}\int^{t}E_{k+\lambda t}d\tau} \tag{2.15}$$

The remainder term is zero for the case when no electric field is present $(\lambda = 0)$, and is zero when $\nabla u_{k+\lambda t} = 0$ for the free electron case [Ref. 7]. In the case where λ or $\nabla u_{k+\lambda t}$ are not zero, but their product is very small, Houston [Ref. 7] claimed (2.14) is a good approximate solution to (2.3). In the case where the remainder is not small, Houston [Ref. 7] showed that the electron wave function can be written as an infinite sum of orthogonal Bloch eigenfunctions:

$$\psi(x,t) = \sum_{l} a_{l}(t)u_{k+2\pi\bar{l}+\lambda t}(x)e^{i(k+2\pi\bar{l}+\lambda t)}e^{-\frac{i}{\hbar}\int^{t}E_{k+2\pi\bar{l}+\lambda t}d\tau} \tag{2.16}$$

where $\bar{l}$ are reciprocal lattice vectors associated with the crystal structure.

Using the method of variation of constants, Houston solved for the time variation of the coefficients $a_l(t)$. Having solved this, he showed [Ref. 7] that the probability for the electron to transition across a Brillouin zone boundary is:

$$P = 4\pi^2 e^{-\alpha} \Big/ \left(1 + e^{-\alpha}\right)^2 \qquad (2.17)$$

where $\alpha = mV^2a^2 \big/ eF\hbar^2$. Houston claims [Ref. 7] this result is similar to Zener's [Ref. 2].

D. GREGORY WANNIER

Wannier's contribution to the field of solid state physics is immense. One of his many contributions was his work on the motion of electrons in solids in the presence of a uniform electric field, and the nature of the energy bands formed by the electric field in that solid. In a series of papers from 1960 to 1968 [Refs. 8-11], Wannier decribed the effects of electric and magnetic fields on electrons in periodic potentials. Wannier's [Ref .8] most significant contribution was to show, for a single band Hamiltonian, that the energy levels of a solid under the effect of an electric field become discretized such that they are a function of the lattice repeat distance a :

$$E_n = \frac{a}{2\pi} \int_0^{\pi/a} W_q(k)dk + nFa \qquad (2.18)$$

where [Ref. 9] E_n are the energy levels, the integral term is the mean energy of the band, and nFa are the ladder spacing intervals. This series of equally spaced energy levels is termed the Stark ladder, or sometimes the Wannier-Stark ladder. The basic idea behind the Stark ladder is that the electric field destroys the degeneracy of the atomic energies of the solid that form the bands. Thus, in Wannier's picture, electric field destroys the zero-field energy bands and replaces them with a ladder of equally spaced energy levels. The existence of Stark ladders in solids has itself been as controversial a topic as Bloch

oscillations, and Stark ladders were first observed in semiconductor superlattices for a single band beginning in the 1980's [Ref. 12]. Wannier also showed [Ref. 10] that if the electron wave function is comprised of Bloch functions, then the energy bands are decoupled, which supports his idea of a discrete energy bands.

Perhaps Wannier's most widely known contribution to solid state physics are the "Wannier functions," which are in essence a Fourier transform of the Bloch states [Ref. 13]. Whereas Bloch states are extended states, i.e., the electron can be found over the entire crystal, the Wannier functions are localized to within a few lattice sites. It can be shown that Wannier functions centered about different lattice sites are orthogonal [Ref. 13]. Also, it was proved that Wannier functions at the same lattice site, but representing different energy bands are orthogonal [Ref. 13]. The Wannier functions are thus a convenient basis set with which to represent the electron wave function.

E. J. ZAK

Zak has written a great deal on the subject of electron motion in periodic potentials under the influence of external electric and magnetic fields. Probably his most outstanding contribution to this field is the derivation and use of a Bloch-type set of functions which are expressible as localized Wannier functions [Ref. 14]. The representation of these functions is known as the kq representation [Ref. 15], and was derived using the fact that finite vector translations in real and reciprocal space in a lattice form a complete set of commuting observables. The difference between his set of functions and normal Bloch-type functions used to solve solid state problems is that the former is a function of two continuous variables k and q, while the latter are function of a discrete band index n and continuous wave vector k [Ref. 15]. He was an outspoken critic, however, of the idea of a Stark ladder in a solid [Ref. 16]. His main criticism was that Wannier's derivation was an approximation using perturbation on a one band Hamiltonian [Ref. 8], and, using the exact time independent Schrodinger equation, Zak showed the integral term of (2.19) was, in fact, an arbitrary constant, thus invalidating the

idea of a ladder of energy levels. Wannier's reply [Ref. 17] was to show that the integral term was valid, and that Stark ladders were a valid model. Zak's reply to Wannier [Ref. 18] was that Wannier still uses an approximate method, and his kq approach is correct. Finally, Zak [Ref. 19] claims, with a more robust proof, that the energy spectrum for a Bloch electron in an electric field is continuous. The author, thus far, has not been able to determine which approach is correct. Multi-band Stark levels are the electrical analog to Landau levels in a magnetic field, and ultimately must be proved or disproved by experimentalists.

F. A. RABINOVITCH

Rabinovitch's first comment [Ref. 20] on the effect of an electric field on an electron in a solid concerned the translational symmetry argument in finite crystals. Rabinovitch [Ref. 20] showed Born-von Karman periodic boundary conditions for finite crystals in an electric field are incompatible with the Schrodinger equation; that is, they do not lead to the expected Stark ladder result for the energy levels. He [Ref. 20] also showed any boundary condition compatible with the Schrodinger equation breaks translational symmetry, and prevents the use of Bloch electron functions. His other works are collaborations with Zak [Refs. 21-22]. In [Ref. 22], using Zak's kq representation for the Schrodinger equation, and using an identical single band approximation as Houston, Rabinovitch and Zak were able to derive the same result as Houston (2.15) for the electron wave function. They argued, since this single band approximation ignores other bands and interband coupling, Houston's solution is unphysical and meaningless. Also, they proposed that an electron composed of the wave function in (2.15) would **only** oscillate with time faster than $2\pi\hbar/eFa$, and thus Bloch oscillations cannot exist.

G. J. N. CHURCHILL AND F. E. HOLMSTROM

In a series of three papers [Refs. 23-25], Churchill and Holmstrom comment on the subject of Bloch oscillations and electron motion in periodic potentials subject to a uniform electric field. They agree with Rabinovitch and Zak's criticism's of this phenomenon [Ref. 22], and using Ehrenfest's theorem, attempt to show why Bloch oscillations could not occur. They consider the following Hamiltonian of the system:

$$H = p^2/2m + \lambda V(x) + eFx \qquad (2.19)$$

where λ is a constant which does not affect the spatial distribution of the lattice potential $V(x)$. They attempt to apply Ehrenfest's theorem to (2.19) [Ref. 23] and derive the acceleration for the electron:

$$d^2\langle x\rangle/dt^2 = \langle -\nabla[\lambda V(x) + eFx]\rangle = -eF + \lambda\langle -\nabla V\rangle \qquad (2.20)$$

By showing a **negative** (non-zero) constant term $(-eF)$ in the acceleration, Churchill and Holmstrom claim [Ref. 23] the velocity must decrease with time, and thus, Bloch oscillations cannot occur. Churchill and Holmstrom did not show the derivation of this result. The author of this thesis believes this result may be incorrect, for they did not show that Ehrenfest's theorem was applied to a wave function in a Bloch state (2.1). Also, they did not specify the periodicity of the potential $V(x) = V(x+a)$. Their result appears so general as to apply to any particle accelerated by an electric field in any general potential, and it can be shown there are many instances where (2.20) is incorrect, e.g., a proton accelerated by an electric field under the influence of gravity.

In another paper [Ref. 24], Churchill and Holmstrom build the electron wave function using eigenstates assuming, *a priori*, that the energy states are in the form of a Stark ladder. They show [Ref. 21] that their Bloch-type wave functions do not approach conventional zero field $(F = 0)$ Bloch states. Later analysis by Krieger and Iafrate [Ref.

23] show this to be the fault with their analysis and later conclusions. (Note: Other analyses by other researchers of Bloch oscillations show that as $F \to 0$, the electron remains in a Bloch state [Refs. 8-11, 14-15, 21-22, 26]) Their final conclusion, again, is that Bloch oscillations do not exist, but that "... accelerated Bloch states can be looked upon as either a type of standing wave or produced as an interference of a stream of electrons moving in the $+x$ direction and a stream moving in the $-x$ direction." [Ref. 24]. In 1991 [Ref. 25], they attempt to refute Krieger and Iafrate's criticisms of previous work [Refs. 23-24], and show that Bloch oscillations exist in free space. Based on their proof [Ref. 25], they conclude that Bloch oscillations cannot exist in a solid if they exist in free space. The author of this paper believes their conclusion is incorrect.

H. J. B. KRIEGER AND G. J. IAFRATE

In 1985, Krieger and Iafrate [Ref. 26] summed up the criticisms [Refs. 14-16, 20-25] of the previous analytical solutions to Bloch oscillations by Zak, Rabinovitch, Churchill and Holmstrom. According to Krieger and Iafrate [Ref. 26], the criticisms can be summarized as follows:

1. The energy eigenvalues of the time independent Schrodinger equation are not quantized but are continuous with all values of E_n allowed.

2. Since the Hamiltonian is not periodic on the boundaries of a (finite) crystal, it is not clear that one can employ the crystal momentum representation of Houston functions since Bloch functions are periodic on the boundary, i.e., a superposition of Bloch functions to represent the wave function ψ will automatically yield a ψ which is periodic on the boundary, but the solution of the time-dependent Schrodinger equation, including the non-periodic scalar potential, $\phi = -eEx$ may not have that property.

3. The crystal momentum representation of the operator x which enters in the calculation may not be well defined because $x\phi_{nk}$ cannot be represented as a linear combination of Bloch states, i.e., $\int |x\phi_{nk}|^2 \, d\tau$ diverges as the crystal approaches the infinite extent in the x direction.

Krieger and Iafrate approach the solution of the time evolution of electrons in an electric field slightly different. Instead of using the familiar scalar potential for the electric field, the chose [Ref. 26] to represent it as a vector potential which is a function of time. The time dependent Schrodinger equation as solved by Krieger and Iafrate is:

$$H\psi(x,t) = \left[\frac{(p-(e/c)\bar{A})^2}{2m} + V(x)\right]\psi(x,t) = i\hbar\frac{\partial\psi(x,t)}{\partial t} \qquad (2.21)$$

where $\bar{A} = \int_0^t \mathcal{E}(t')dt'$, and $\mathcal{E}(t)$ is an electric field turned on at time $t = 0$.

The eigenfunctions [Ref. 26] are solved from following equation:

$$\left[\frac{(p^2-(e/c)\bar{A})^2}{2m} + V(x)\right]\phi_i'(x,t) = \varepsilon_i(t)\phi_i'(x,t). \qquad (2.22)$$

Using a gauge transformation [Ref. 26], the solution of the eigenfunctions are:

$$\phi_i'(x,t) = e^{ieAx/\hbar c}\phi_{n,k}(x), \qquad (2.23)$$

Expanding the wavefunction $\psi(x,t)$ as a sum of eigenfunctions in Eq (2.24), and solving for the time variation of the expansion coefficients, $\dot{a}_n(t)$, of the eigenfunctions, Krieger and Iafrate [Ref. 26] reach the same result as Houston [Ref. 7] did:

$$\dot{a}(t) = \frac{F(t)}{i\hbar}\sum_{n'} a_{n'}(t)X_{nn'}(k(t))e^{\frac{i}{\hbar}\int_0^t [\varepsilon_n(k(t'))-\varepsilon_{n'}(k(t'))]dt'}. \qquad (2.24)$$

Zak [Ref. 27] criticized this formulation, and claimed this solution was incorrect due to the wave function repeating itself at every time on every lattice cell. He concludes the basis set (2.24) is incorrect, and that Krieger and Iafrate moved the problems of spatial periodicity into the time domain. Krieger and Iafrate's rebuttal [Ref. 28], agree that their basis states are periodic in time at lattice sites, but disagree with his conclusions concerning this fact. They show for any lattice site that the wave function repeats itself at

the Bloch repeat time, not just any time as Zak [Ref. 27] assumes. Also, they show in Zak's derivation that he actually uses a different Hamiltonian than they do [Ref. 28], and seem to overcome previous objections with boundary conditions [Refs. 14-16, 20-25] using their expansion on basis states based on the vector potential derivation.

I. L. ESAKI AND R. TSU

Esaki and Tsu, in 1970, predicted that Bloch oscillations might be seen in a structure called a "semiconductor superlattice" [Ref. 3]. Given the state of art in semiconductor fabrication, it would be possible to grow layers of different material in a way that a periodic band structure would be created. Given the probability of Zener interband tunneling, Esaki and Tsu [Ref. 3] said that if the scattering times were long, Terahertz (THz) oscillations would be possible, and the electron would undergo reflections at miniband boundaries [Brillouin Zone]. The typical numbers needed, as estimated by Esaki and Tsu for frequency υ_B = 250 GHz, $F = 10^3 V/cm$, and a = 10 nm, with the scattering time greater than four picoseconds. This article was the first in which the possibility was raised of creating a structure in which radiation from an electron undergoing Bloch oscillations might be obtained.

J. D. EMIN AND C. F. HART

In 1988, Emin and Hart [Ref. 29] commented on the time evolution of electrons in a periodic potential under the influence of an external electric field. Their novel approach showed that the applied electric field can be broken up as a sum of a periodic function (sawtooth), and non-periodic (ladder), and that in their multiband solution, the ladder forms the basis of the Stark ladder of multiband energy eigenstates [Ref. 29]. Using a modification of Krieger and Iafrate's approach [Ref. 26], they derive an equation of motion where their Bloch eigenstates are a function of the periodic portion of the electric

field [Ref. 29]. Since then, the Emin-Hart approach has been shown by several authors to be incorrect [Refs. 30-32].

K. M. LUBAN AND A. BOUCHARD

In 1993, Luban and Bouchard [Ref. 5], using highly accurate numerical techniques, simulated the motion of an electron wavepacket in a semiconductor superlattice under the influence of an electric field. The advantage of their approach was the numerical simulation contained all powers of the Hamiltonian containing all energy bands, instead of single band Hamiltonian approximations used by previous analytical approaches. Coinciding with recent four wavemixing experiments which detected Bloch radiation for the first time from superlattices [Ref. 4], Luban and Bouchard's numerical simulations clearly demonstrated (absent scattering events) that an electron will undergo Bloch oscillations in a semiconductor superlattice, and for the first time, showed that Bloch oscillations are a bona-fide aspect of the dynamics of independent electrons in a solid.

III. NUMERICAL METHODS

A. TIME DEPENDENT SCHRODINGER EQUATION (TDSE)

Solving the Time Dependent Schrodinger Equation is essential to the modeling of Bloch oscillations. The general one dimensional Schrodinger equation is:

$$-\frac{\hbar^2}{2m}\frac{\partial^2 \psi(x,t)}{\partial x^2} + V(x,t)\psi(x,t) = i\hbar\frac{\partial \psi(x,t)}{\partial t}, \tag{3.1}$$

where $\psi(x,t)$ is the wave function of the electron, and $V(x,t)$ is the potential energy function of the electron. We will consider a system in which $V(x,t)$ is independent of time, thus making V a function of position only. The Hamiltonian of a system is defined as $H = T + V$, where T is the kinetic energy operator, and V is the potential seen by the electron. The Schrodinger equation can be cast in terms of the Hamiltonian operator. If the momentum operator p is given by $\frac{\hbar}{i}\frac{\partial}{\partial x}$, then the Schrodinger equation can be cast in the form of an operator equation, with $H = \frac{p^2}{2m} + V$. The time dependent Schrodinger equation reads:

$$H\psi(x,t) = i\hbar\frac{\partial \psi(x,t)}{\partial t} \tag{3.2}$$

To solve this numerically, one must discretize (3.2). We will discuss the discretization process in the following sub-sections.

1. Discretization of the Wave Function

First, we represent the continous variable x as a discrete variable, $x = x_0 + n\Delta x$, where Δx is the mesh size, x_0 is the starting value, and n is any integer. Also, we represent time as a discrete variable, $t = t_0 + m\Delta t$, where Δt is the time mesh size, t_0 is the initial time, and m is any integer. The initial points, x_0, t_0 are both set equal to zero to simplify the scheme. Also, this form of discretization for time allows the efficient use of a loop in a computer program. The form of our sampled wave function is a column vector, with each sample being taken at a mesh point, such that for any time t, the wave function will look like:

$$\psi_{m\Delta t}(x) = \begin{bmatrix} \psi(\Delta x) \\ \psi(2\Delta x) \\ \vdots \\ \psi((N-1)\Delta x) \\ \psi(N\Delta x) \end{bmatrix} \tag{3.3}$$

where N is the total number of mesh points in the discretization. Using a loop over time, the computer program generates a new ψ vector for each time step.

2. Discretization of the Hamiltonian

The Hamiltonian has two terms: the kinetic energy operator $T = -\dfrac{\hbar^2}{2m}\dfrac{\partial^2}{\partial x^2}$, and the potential $V(x)$. We must find a suitable discrete representation for each term. The discrete representation of the potential is easy.

Being a function of x, it takes on the same form as the wave function, i.e., a column vector such that:

$$V(x) = \begin{bmatrix} V(\Delta x) \\ V(2\Delta x) \\ \vdots \\ V((N-1)\Delta x) \\ V(N\Delta x) \end{bmatrix}.$$ (3.4)

The discretization of the kinetic energy operator is more involved. A suitable discrete representation for the second spatial derivative must be found. To approximate it, we look at the Taylor series expansion for arbitrary functions $f(x + \Delta x)$ and $f(x - \Delta x)$:

$$f(x + \Delta x) = f(x) + \frac{1}{1!} \frac{df(x)}{dx} \Delta x + \frac{1}{2!} \frac{d^2 f(x)}{dx^2} \Delta x^2 + \dots$$ (3.5)

and

$$f(x - \Delta x) = f(x) - \frac{1}{1!} \frac{df(x)}{dx} \Delta x + \frac{1}{2!} \frac{d^2 f(x)}{dx^2} \Delta x^2 + \dots$$ (3.6)

Ignoring terms higher than order two, and taking the sum of (3.5) and (3.6), we find that

$$\frac{d^2 f(x)}{dx^2} = \frac{f(x + \Delta x) + f(x - \Delta x) - 2f(x)}{\Delta x^2}$$ (3.7)

Letting the total derivative go to a partial derivative in x, and letting ψ be our arbitrary function f, the kinetic energy operator T acting on ψ for an arbitrary mesh point $n\Delta x$ is:

$$-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} \psi(n\Delta x) = -\frac{\hbar^2}{2m\Delta x^2} [\psi((n+1)\Delta x) + \psi((n-1)\Delta x) - 2\psi(n\Delta x)].$$ (3.8)

Therefore, the Hamiltonian acting on ψ at an arbitrary mesh point $n\Delta x$ has the form:

$$H\psi(n\Delta x) = -\frac{\hbar^2}{2m\Delta x^2}\left[\psi((n+1)\Delta x) + \psi((n-1)\Delta x) - 2\psi(n\Delta x)\right] + V(n\Delta x)\psi(n\Delta x). \qquad (3.9)$$

If our mesh runs from $n = 0,1,2...N$, in solving the the Hamiltonian, it arises that values for $\psi(-1\Delta x)$ and $\psi((N+1)\Delta x)$ are needed. These exist outside the mesh system we are looking at, and therefore are simply set to zero. This is tantamount to assuming the potential suddenly becomes infinite outside the mesh system. This, as a practical consequence, forces one to construct the spatial system sufficiently large so that, over the time scales of interest, the wave functions do not reflect from these "hard walls."

The effect of the discretization is thus to replace a single differential equation with a set of N coupled equations. The form of the Hamiltonian is an $N \ X \ N$ matrix:

$$H = \begin{bmatrix} -2\alpha \div V & \alpha & 0 & \cdots & & 0 \\ \alpha & -2\alpha + V & \alpha & 0 & & \vdots \\ 0 & \ddots & \cdot & \ddots & \ddots & 0 \\ \vdots & & 0 & \alpha & -2\alpha + V & \alpha \\ 0 & \cdots & & 0 & \alpha & -2\alpha + V \end{bmatrix} \qquad (3.10)$$

where $\alpha = -\dfrac{\hbar^2}{2m\Delta x^2}$. It is seen that the Hamiltonian is a tridiagonal matrix, with only the main diagonal and the first upper and lower diagonals having non zero terms. To reduce the amount of space required for computer memory, the computer program in Appendix A uses a sparse representation for storing the Hamiltonian. Instead of an $N \ X \ N$ matrix, we use an $N \ X \ 3$ matrix storing only the non-zero terms:

$$H = \begin{bmatrix} 0 & -2\alpha + V & \alpha \\ \alpha & -2\alpha + V & \alpha \\ \vdots & \vdots & \vdots \\ \alpha & -2\alpha + V & \alpha \\ \alpha & -2\alpha + V & 0 \end{bmatrix} \qquad (3.11)$$

B. SOLUTIONS OF THE TIME DEPENDENT SCHRODINGER EQUATION

Equation (3.2) is a first order differential equation of the time variable. The solution of this first order differential equation has a unique solution, given in the Schrodinger representation by:

$$\psi(x,t) = e^{-\frac{iHt}{\hbar}}\psi(x,0) \tag{3.12}$$

To perform practical computations of $\psi(x,t)$, we must know two things. First, the initial state of the wave function must be known or guessed for time $t = 0$. Secondly, an approximation for $e^{-\frac{iHt}{\hbar}}$ must be made. This value is not only complex, but it is also strictly unitary, and any approximation must maintain unitarity for it to be considered valid. Unitarity means that the normalization of the wave function is constant at all times, and the wave function for any time t must satisfy the following integral equation:

$$\int_{-\infty}^{\infty}\psi^*(x,t)\psi(x,t)dx = 1 \tag{3.13}$$

In the following sub-sections, we will discuss approximation methods and their relative strengths and weaknesses.

1. Power Series Expansion

Numerically calculating the time evolution operator $e^{-\frac{iHt}{\hbar}}$ is not easy. One could use a power series expansion to represent the operator. For an arbitrary operator A, the power series expansion of e^A is:

$$e^A = 1 + A + \frac{A^2}{2!} + \frac{A^3}{3!} + \dots \tag{3.14}$$

Based on this result, the power series expansion of the time evolution operator is:

$$e^{-\frac{iHt}{\hbar}} = 1 - \frac{iHt}{\hbar} - \frac{H^2 t^2}{2\hbar^2} + \frac{iH^3 t^3}{6\hbar^3} + \dots \tag{3.15}$$

A truncation of the expansion can be implemented easily numerically, since it is only a finite sum of products of terms. The restriction that any approximation maintain unitarity and satisfy (3.13) prevents the use of it in program. Any truncation of this infinite series removes the property of unitarity from it, and since a computer cannot generate an infinite amount of terms, any solution generated from the truncation would be invalid.

2. Magnus Expansion

In 1954, Wilhem Magnus derived an expansion which can be used to represent the time evolution operator. Using the Baker-Hausdorff theorem, Magnus derived a solution to the first order differential equation [Ref. 33]:

$$\frac{d}{dt} Y(t) = A(t)Y(t) \tag{3.16}$$

where $Y(t)$ is of the form:

$$Y(t) = e^{\Omega(t)}Y(0) \tag{3.17}$$

and $\Omega(t)$ is:

$$\Omega(t) = \int_0^t A(\tau)d\tau + \frac{1}{2}\left[\int_0^t A(\tau), \int_c^\tau A(\sigma)d\sigma\right]d\tau + \dots \tag{3.18}$$

where the brackets indicate commutators. This result was independently derived by Pechukas and Light [Ref 34]. Applying the Magnus expansion requires a very

sophisticated numerical integration routine, and requires a great deal of error analysis and monitoring of the results to ensure numerical stability and accuracy [Ref. 35]. Because of its complexity, this method was not chosen.

3. Explicit Alogrithm for Solving the TDSE

In 1991, P. B. Visscher developed an explicit numerical algorithm to solve the time depedent Schrodinger equation [Ref. 36]. Starting with equation (3.1), Visscher rewrote it in terms of solutions of the real and imaginary portions of the wave function such that:

$$\frac{d\psi_r(x,t)}{dt} = H\psi_i(x,t) \tag{3.19}$$

and

$$\frac{d\psi_i(x,t)}{dt} = -H\psi_r(x,t) \tag{3.20}$$

where $\psi_r(x,t)$ is the real portion of the wave function, and $\psi_i(x,t)$ is the imaginary portion of the wave function [Ref. 36]. He claims this approach is the same as calculating a trajectory, and thus in the discretization of each equation, each portion is defined at staggered times. For the real portion of the wave function $\psi_r(x,t)$, it is defined at times equal to $t = 0, \Delta t, 2\Delta t, \ldots$, while the imaginary portion is defined at times $t = 0.5\Delta t, 1.5\Delta t, 2.5\Delta t, \ldots$ [Ref. 36]. The discretization of equations (3.19) and (3.20) is:

$$\psi_r(x, t + 0.5\Delta t) = \psi_r(x, t - 0.5\Delta t) + \Delta t H\psi_i(x,t) \tag{3.21}$$

and

$$\psi_i(x, t + 0.5\Delta t) = \psi_i(x, t - 0.5\Delta t) - \Delta t H\psi_r(x,t) \tag{3.22}$$

To start the iteration, initial values for $\psi_r(x,0)$ and $\psi_i(x,0.5\Delta t)$ must be obtained, and time must start at $t = 0.5\Delta t$ [Ref. 36]. Visscher also points out that because the real and imaginary portions of the wave function exist at different time steps, calculating the overall probability density could be problematic. A set of equations which conserve probability for integer and half integer units of time are:

$$|\psi(x,t)|^2 = \psi_r(x,t)^2 + \psi_i(x,t+0.5\Delta t)\psi_i(x,t-0.5\Delta t) \tag{3.23}$$

for integer time intervals, and for half integer time intervals:

$$|\psi(x,t)|^2 = \psi_r(x,t+0.5\Delta t)\psi_r(x,t-0.5\Delta t) + \psi_i(x,t)^2 \tag{3.24}$$

This scheme is second order accurate, and conserves probability, satisfying equation (3.13). The claim of Visscher is this scheme is three times faster than the actual scheme used by the author of this thesis (Cayley method). This paper was discovered in the process of the thesis write-up, and therefore this method and its author's claims could not be compared to the Cayley method. If Visscher's claim is true, then it would be an outstanding method to use, and would be an excellent model for future students to use.

4. Cayley Hamilton Approximation

The approximation actually used for the time evolution operator is the Cayley-Hamilton approximation [Refs. 37,38]. It is Hermitean, and maintains unitarity, as well as has good properties for keeping error low. The Cayley approximation of the time evolution operator is given by:

$$e^{-\frac{iH\Delta t}{\hbar}} = \frac{1 - \frac{1}{2\hbar}iH\Delta t}{1 \div \frac{1}{2\hbar}iH\Delta t} \tag{3.25}$$

which has error on the order of $(\Delta t)^3$. This error can be seen when compared to the power series expansion of $e^{-\frac{iH\Delta t}{\hbar}}$. Taking the first four terms in the power series expansion of this time evolution operator from (3.14):

$$e^{-\frac{iH\Delta t}{\hbar}} = 1 - \frac{iH\Delta t}{\hbar} - \frac{(H\Delta t)^2}{2\hbar^2} + i\frac{(H\Delta t)^3}{6\hbar^3} + \ldots, \tag{3.26}$$

while the expansion for the approximation $\dfrac{1 - \frac{1}{2\hbar}iH\Delta t}{1 + \frac{1}{2\hbar}iH\Delta t}$ is:

$$\frac{1 - \frac{1}{2\hbar}iH\Delta t}{1 + \frac{1}{2\hbar}iH\Delta t} = 1 - \frac{iH\Delta t}{\hbar} - \frac{(H\Delta t)^2}{2\hbar^2} + \frac{i(H\Delta t)^3}{4\hbar^3} + \ldots \tag{3.27}$$

these two expansions differ beginning only in the third term, so the error will be third order. The Cayley approximation to the original solution is:

$$\psi(x, t + \Delta t) = \frac{1 - \frac{1}{2\hbar}iH\Delta t}{1 + \frac{1}{2\hbar}iH\Delta t}\psi(x, t) \tag{3.28}$$

Finally, the computer will iterate the following algorithm:

$$(1 + \tfrac{1}{2\hbar}iH\Delta t)\psi(x, t + \Delta t) = (1 - \tfrac{1}{2\hbar}iH\Delta t)\psi(x, t) \tag{3.29}$$

In numerical analysis, this type of solution is called an "implicit" scheme or a Crank-Nicholson scheme [Ref. 38].

C. SOLVING THE CAYLEY APPROXIMATION

Equation (3.29) has the form:

$$M^*\psi(x, t + \Delta t) = M\psi(x, t) \tag{3.30}$$

where $M = I + \dfrac{i\Delta t}{2\hbar} H$, and I is the identity matrix, and H is an $N \times N$ matrix.

Solving for the wave function at the next time step is the ultimate goal in order to model the time varying motion of the electron. There are several methods of solving equation (3.29) available, and the methods will be discussed in the following sub-sections.

1. Solution by Inversion

The most direct solution of equation (3.30) for $\psi(x, t + \Delta t)$ is:

$$\psi(x, t + \Delta t) = (M^*)^{-1} M \psi(x, t) \tag{3.31}$$

but it is numerically intensive. M^* is a tridiagonal matrix, while the inverse, $(M^*)^{-1}$, is a full matrix, and must be solved before proceeding to solve equation (3.31). The inverse can be obtained by several methods (Gaussian reduction, Gauss Jordan elimination, etc...), but the ultimate solution of equation (3.31) takes an order of N^3 operations to solve [Ref. 38] if $(M^*)^{-1}$ and M are $N \times N$ matrices. There is a more elegant method which takes advantage of the tridiagonal nature of M and M^*, and reduces the number of operations to the order of N. This is the L-U decomposition method, and will be discussed in detail next.

2. L-U Decomposition

This method of solving a linear equation was taken from *Numerical Recipes in C* [Ref.]. Equation (3.30) has the form $A \cdot x = b$, where b is an $N \times 1$ column vector and is the solution of $[I - \frac{i\Delta t}{2\hbar} H] \psi(x, t)$. $A = [I + \frac{i\Delta t}{2\hbar} H] = M^*$, and x is what we are solving for: $\psi(x, t + \Delta t)$.

In order to solve this by L-U decomposition, we break A up into two matrices such that:

$$A \cdot x = (L \cdot U) \cdot x = L \cdot (U \cdot x) = b.$$ (3.32)

We solve this by back substitution, first solving for an intermediate vector y, such that $L \cdot y = b$, and then back solve $U \cdot x = y$. This involves solving a set of N linearly independent equations. In decomposing a tridiagonal matrix, L takes on the form:

$$L = \begin{bmatrix} \alpha_{11} & 0 & \cdots & & 0 \\ \alpha_{21} & \alpha_{22} & & & \vdots \\ 0 & \ddots & \ddots & & \\ \vdots & & \alpha_{N-2,N-1} & \alpha_{N-1,N-1} & 0 \\ 0 & \cdots & 0 & \alpha_{N-1,N} & \alpha_{NN} \end{bmatrix}$$ (3.33)

where α_{ij} are the coefficients of the L matrix. In order to conserve computer storage memeory, the program in the Appendix stored the L matrix in an $N \times 2$, which only held the non-zero elements, so that L is:

$$L = \begin{bmatrix} \alpha_{11} & 0 \\ \alpha_{21} & \alpha_{22} \\ \vdots & \vdots \\ \alpha_{N-2,N-1} & \alpha_{N-1,N-1} \\ \alpha_{N-1,N} & \alpha_{NN} \end{bmatrix}$$ (3.34)

Likewise, the U matrix was handled in a similar fashion. The form of the U matrix when derived from a tridiagonal matrix is:

$$U = \begin{bmatrix} \beta_{11} & \beta_{12} & 0 & \cdots & & 0 \\ 0 & \beta_{22} & \beta_{23} & & & \vdots \\ \vdots & & \ddots & \ddots & & 0 \\ & & & \beta_{N-1,N-1} & \beta_{N-1,N} \\ 0 & \cdots & & 0 & \beta_{NN} \end{bmatrix}$$ (3.35)

where β_{ij} are the coefficients of the U matrix.

Again, to conserve space, U was actually stored in an $N \times 2$ matrix and takes almost the same form as L :

$$U = \begin{bmatrix} \beta_{11} & \beta_{12} \\ \beta_{22} & \beta_{23} \\ \vdots & \vdots \\ \beta_{N-1,N-1} & \beta_{N-1,N} \\ 0 & \beta_N \end{bmatrix} \tag{3.36}$$

The method of solution is straight forward. First, all the coefficients of the L and U matrices must be solved. Then equation (3.32) can be solved in two steps. The first step is to solve for $L \cdot y = b$, which can be done as follows:

$$y_1 = \frac{b_1}{\alpha_{11}}$$

$$y_i = \frac{1}{\alpha_{ii}} \left[b_i - \sum_{j=1}^{i-1} \alpha_{ij} y_j \right] \text{ for } i = 2,3,\ldots,N \tag{3.37}$$

This procedure is accomplished very quickly due to the tridiagonal nature of the L matrix. Then to solve for x, the final answer, it is solved by back substitution as follows:

$$x_N = \frac{y_N}{\beta_{NN}}$$

$$x_i = \frac{1}{\beta_{ii}} \left[y_i - \sum_{j=i+1}^{N} \beta_{ij} x_j \right] \text{ for } i = N-1, N-2,\ldots,1 \tag{3.38}$$

Once this answer for the wave function for the new time step is obtained, it is multiplied by M to form a new b vector, and the process is repeated to solve for the wave function at the next time step. This process is repeated in a loop over the time of the simulation. Results of the program will be discussed in the next chapter.

IV. RESULTS AND CONCLUSIONS

The computer code in the Appendix has been under development for nearly a year. The solution of the time dependent Schrodinger equation using the Cayley approximation sounds easy to accomplish numerically, but has been challenging to successfully accomplish. C language was chosen due to the local support and our familiarity with it. Since the electron wave function is complex, solving the time dependent Schrodinger equation numerically required the use of a user defined structure. All variables were defined of type complex, with a real and imaginary part of double precision. The first efforts in developing the code were writing reliable functions to add, subtract, multiply, divide, and conjugate complex numbers. These tasks were verified using simple algebraic equations that the author programmed and knew the results ahead of time. The functions performed as expected.

The next step was to write a routine that would perform an L-U decomposition on an N X N matrix. The concepts were well laid out in *Numerical Recipes in C* [Ref. 38], but tailoring it a tridiagonal matrix was more difficult than expected. After several attempts, C code was written to perform the L-U decomposition, and results of our decomposition routine on a general N X N matrix were verified against an identical matrrix using MATLAB's L-U decomposition function. The decomposed matrices were identical. Finally, the back substitution routine was written to solve the time dependent Schrodinger equation (3.29) using the Cayley approximation. To ensure our code was accurate, our first model was a one dimensional free particle, with $V = 0$. The wave packet for this model, and all subsequent simulations was a normalized Gaussian wave packet $\psi(x) = Ce^{-\frac{x^2}{2\sigma}}$, where C is a normalization constant, and σ controls the width of the packet. The free particle model behaved as expected, with the wave packet spreading out in both the $+x$ and $-x$ directions. To ensure our numerical model was correct, another system simulated was an electron wave packet in a harmonic oscillator potential $V = \frac{1}{2}m\omega^2 x^2$. The response of the particle should be to diffuse out, and gather itself back

at exact time intervals of $2\pi/\omega$. The model again showed the wave packet evolve as expected, and repeat at exact time intervals of $2\pi/\omega$.

Confident that the model to numerically simulate the time dependent Schrodinger equation was accurate, electron wave packets in periodic potentials with an external electric field applied were modeled. The simulations were ran either on a Sun Sparcstation 20, or a Cray C-90 super-computer at Wright Patterson AFB. For problems modeling Bloch oscillations, the Sparcstation typically took 12 hours to run, while the super-computer would take eight hours. A variety of results were generated, and a representative sample is presented and discussed below:

A. NON LOCALIZED WAVE PACKET IN GENERAL POTENTIAL

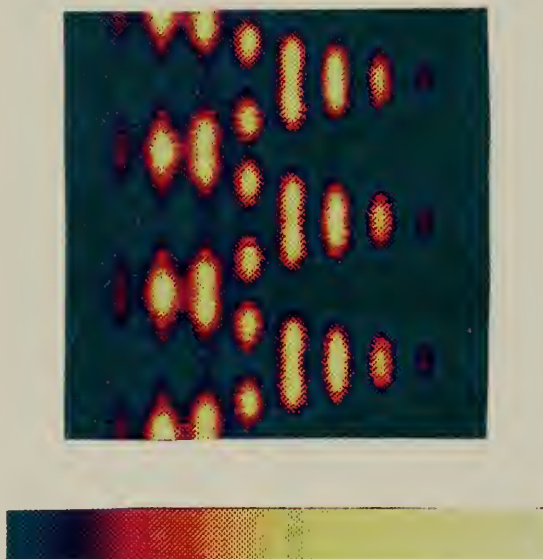Figure (1) is a picture of an electron clearly undergoing Bloch oscillations.

Figure (1). Electron Undergoing Bloch Oscillations

For all simulation output, the vertical axis represents time, with the electron wave packet starting at the top of the figure working its way down in time, and the horizontal axis of

the figure is space. The color bar at the bottom of the figure shows the relative probability, with zero probability being green, and maximum probability being yellow, with a continuous color scale showing probabilities in between. The horizontal scale is 10 nm, and the amplitude of oscillation being nearly that large. For the system in Figure (1), the potential function is given by $V = 0.5|\cos(2x)|$, with $a = \pi/2$ nm being the repeat distance. The applied electric field strength is $F = 10^5\,V/cm$. Given the previous parameters, the Bloch repeat time is $\tau_B = \frac{h}{eFa} = 264\,fs$. The code was run for 16000 time steps, which generated three oscillations. It is clear the center of mass of the electron is oscillating back and forth, and thus, we would expect to radiate like a classical dipole. No other dynamic electron effects are seen here, so, by accident, we chose a system that would undergo perfect Bloch oscillations instead of executing interband transitions or remaining in a stationary state. Without calculating the energy bands and eigenvectors and composing the inital state of the electron as a superposition of eigenfunctions of a single band (Wannier functions), the behavior could not be exactly predicted prior to running the code.

B. LOCALIZED ELECTRON IN A GENERAL POTENTIAL

Figure (2) is a picture of an electron undergoing a "breathing mode" of oscillation.
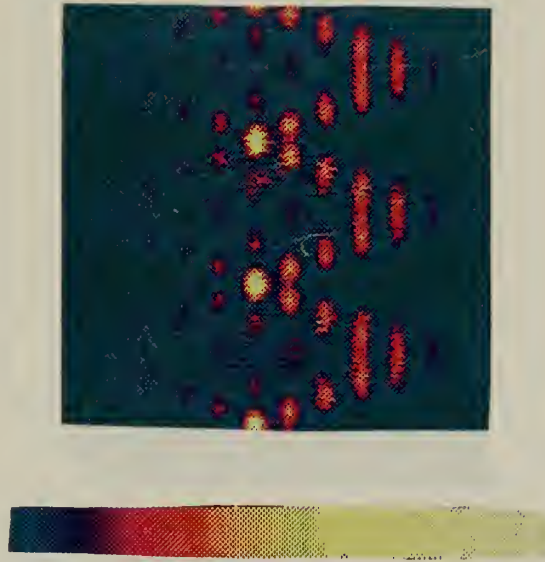

Figure (2). Electron in a "Breathing Mode"

The system is exactly the same as previous, with the only difference being that the electron wave packet is localized in a well. We did this by reducing σ, which controls the width of the wave packet. Instead of executing center of mass oscillations, the electron wave packet "breathed" in and out at the Bloch frequency. The electron preferentially breathed in the direction of lower energy. The code was run for 16000 time steps, showing three breathing modes. This phenomenon would not radiate, because, as seen in the picture, the average center of mass does not appreciably move over time. This phenomenon was actually predicted by Zener in 1933 [Ref. 2], and his explanation is the electron is localized near the Brillouin zone boundary, and it only transitions between $k = +\frac{\pi}{a}$ and $k = -\frac{\pi}{a}$ in k space by Bragg reflection, thus executing a "breathing" in real space.

C. ELECTRON REFLECTIONS AT BOUNDARIES

Figure (3) is an example of electron wave packet reflection off the boundaries of the system investigated:
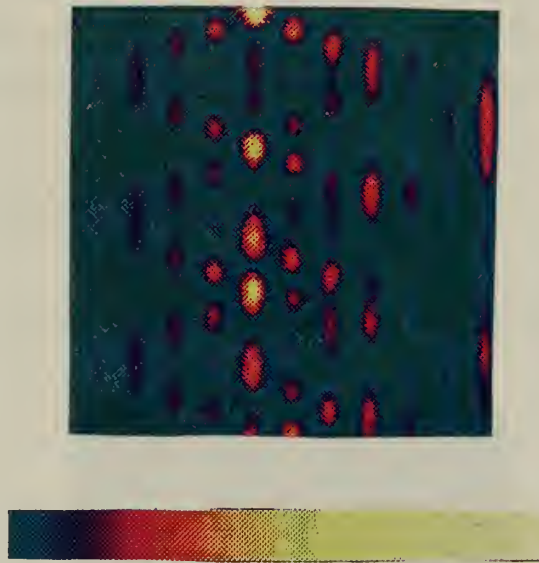

Figure (3). Electron Reflection of Boundaries

In the process of discretizing the time dependent Schrodinger equation, it imposes finite boundaries on the system. The effect of reaching a boundary, as seen in Figure (3), is quite dramatic. The wave reflects perfectly off the boundary, and begins to interfere with the rest of the wave function executing a Bloch "breathing" oscillation. After several reflections, the "breathing" becomes completely distorted, as the wave function folds over on the right side. For future simulations, a test could be developed to determine if the wave function was near a boundary, and the test would stop the simulation if a reflection occurred.

D. KRONNIG-PENNY SIMULATIONS

The Kronnig-Penny one dimensional square wave potential is an excellent model to simulate the conduction band edge of a general semiconductor superlattice. The superlattice simulated is a GaAs/Al$_{0.3}$Ga$_{0.7}$As superlattice, with barrier height equal to 0.243 eV. In the following sections, we will discuss the effect of varying different parameters, and their effect of the motion of the electron in the lattice.

1. Non-localized Electron in a Superlattice

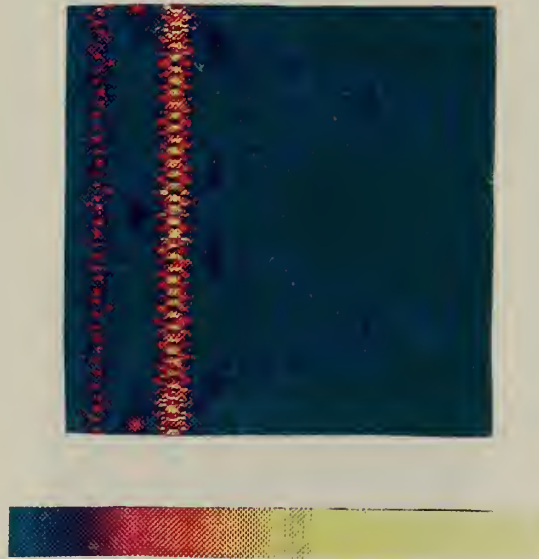Figure (4) is a picture of an electron in a superlattice potential:

Figure (4). Non-localized Electron in a Superlattice

The potential function is given by $V = 0.243$ eV for the Al$_{0.3}$Ga$_{0.7}$As barriers, $V = 0$ eV for the GaAs barriers, and $a = 10$ nm being the repeat distance. The AlGaAs barriers were 5.1 nm thick, and the GaAs barriers were 4.9 nm thick. The applied electric field

strength is $F = 10^4\,V/cm$. Given the previous parameters, the Bloch repeat time is $\tau_B = \frac{h}{eFa} = 827\,fs$, and the amplitude of oscillation was approximately 20 nm. The simulation was run for 17000 time steps, giving two oscillation periods to observe. The electron wave packet was approximately 250 angstroms wide. It is seen part of the electron is "ripped away" and undergoes Bloch oscillations, and parts of it bifurcate and tunnel through the barriers, remaining relatively stationary. This electron is clearly in a superposition of a dynamic and stationary state. The electron is undergoing Bloch oscillations, but it could also be transistioning energy bands or remaining in the ground state. Without calculating energy band transition probabilities, it is impossible to tell in this calculation. That could and should be built into a more sophisticated model.

2. Effect of Varying Repeat Distance

Figure (5) is a picture of an electron in a superlattice with half the repeat distance of the electron in section 1:
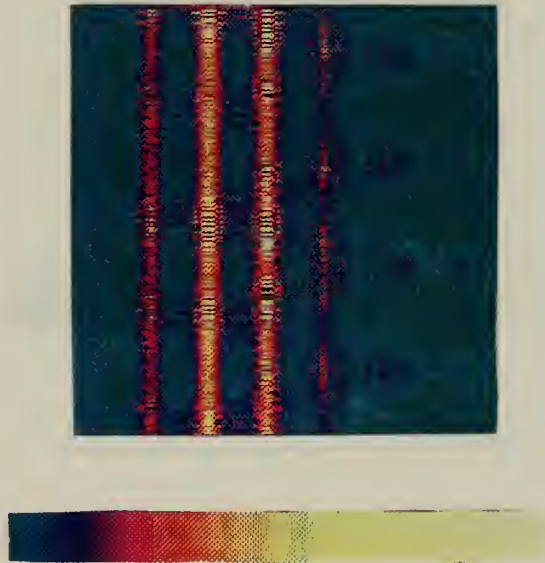

Figure (5). Electron in Superlattice (Differing Repeat Distance)

The repeat distance was changed from the system in section 1 from $10\ nm$ to $5\ nm$. Keeping the electric field constant, this changes the repeat time to $\tau_B = \frac{h}{eFa} = 413.5\ fs$. The simulation was run for 17000 time steps, showing four oscillation periods. The result is much the same as the previous two before, except the electron tunnels through more barriers, and less of it is available for Bloch oscillations, which are faintly present.

3. Effect of Varying Barrier Thickness

Figure (6) shows the effect of changing the system in section 2 by reducing the width of the AlGaAs barriers, and increasing the GaAs well width such that the $5\ nm$ repeat distance is maintained:
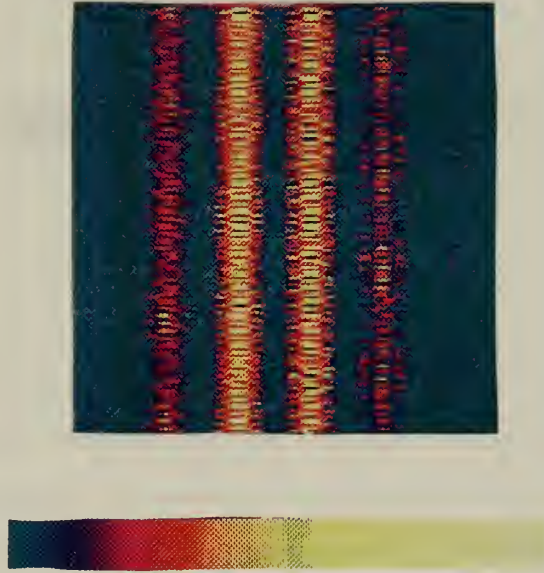

Figure (6). Electron in a Superlattice (Varying Barrier Width)

The electron completely tunnels through the barriers, and it appears the electron is not undergoing Bloch oscillations at all. This may be because the barriers are relatively thin ($1.5\ nm$), and repeat very closely to one another ($5\ nm$).

4. Effect of Varying Electron Mass

Figure (7) is a picture of the effect of changing the electron mass of the system described in section 3:
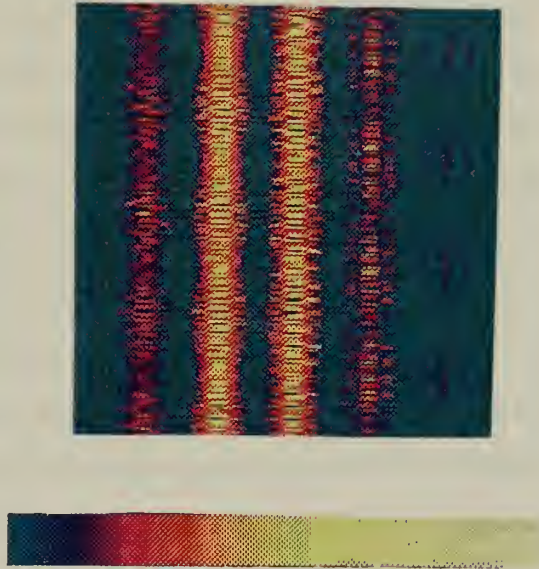

Figure (7). Electron in a Superlattice (Varying Electron Mass)

The mass of the electron in the system in section 5 was changed to 0.85 times the bare electron mass. The effect of making the electron "lighter" was to make Bloch oscillations somewhat apparent, where as they were not in the previous simulation. This represents a physical effect. In a semiconductor, the interaction of an electron with each material can be modeled by changing the electron mass to an effective mass. While the actual effective masses of GaAs and AlGaAs were not used, the simulation is effective in demonstrating the effect of the effective mass approximation in semiconductors, and shows that semiconductors with effectively "light" electrons are ideal materials to stimulate Bloch oscillations where as they might not be present on other materials.

E. SUMMARY

We have demonstrated that Bloch oscillations are a genuine phenomenon of an electron in a periodic potential. The rich variety of dynamic phenoma of Bloch electrons is a great source for further research. There are a wide variety of potential applications for stable GHz and THz oscillators for high speed integrated circuits and Rf sensors. More sophisticated models of this effect can be made such as including the effective mass variation of the layers, calculating the energy eigenvalues and vectors to start the initial state in a single energy band, calculating the effect of the electron motion on the potential using the Poisson equation, and using that potential in the Schrodinger equation (self-consistent Poisson-Schrodinger equation), incorporate scattering mechanisms such as electron-electron scattering, electron-hole elimination, electron phonon/photon scattering, and a variety of other mechanisms present in the solid. Including these effects adds to the complexity of the model and code, and would require the immense resources of a super computer, but accurately modeling this effect could reveal new and useful applications for future devices.

APPENDIX: CAYLEY METHOD IN ANSI C

```c
#include <stdio.h>
#include <stdlib.h>
#include <math.h>
#define PI  3.14159265

struct complex {
  double r;
  double c;
};

struct complex Cadd(struct complex x, struct complex y);

struct complex Csub(struct complex x, struct complex y);

struct complex Cmult(struct complex x, struct complex y);

struct complex Cdiv(struct complex x, struct complex y);

struct complex Ceq(struct complex x);

struct complex Cconj(struct complex x);


struct complex C1, C2, M[10002][4], Ms[10002][4], psi[10002];
struct complex npsi[10002], magpsi[10002], one, eye, sum, temp;
struct complex L[10002][3], U[10002][3], y[10002], conj[10002];
struct complex zero, temp1, V[10002], b[10002], psit[10002], magipsi[10002];
struct complex nconj[10002], nmagpsi[10002];

double dt,dx, hbar,m,c1, c2, tconst, sigma, e, F;
int i,j,N;
long loop;

main()

/* Time Dependent Schroedinger Equation - using Cayley method */
/* L-U Decomposition program, code based on procedure in Numerical Recipes*/
/* in C, pp 43-44 */

/* L is alpha units */
/* U is beta units */
```

```
{

N=10001;

m=9.1e-31;          /* Mass of electron in kg */
dt=0.05;            /* Time step in femto seconds */
dx=0.01;
hbar=0.6582;    /* Plancks constant divided by 2 pi in eV fs*/
tconst=0.03810;     /* hbar squared divided by twice mass of electron eV nm2 */
c2=tconst/dx/dx;  /* Constant that wraps up all constants*/
c1=0.5*dt/hbar;    /* second constant that wraps up all constants */
sigma=4000.0;
e=1.0;       /* Charge of electron */
F=1e-2;          /* Field strength in Volts/nm */

C1.r=0.0;
C1.c=1.0*c1;

C2.r=1.0*c2;
C2.c=0.0;

zero.r=0.0;
zero.c=0.0;


one.r=1.0;          /* One - real number */
one.c=0.0;

eye.r=0.0;          /* Imaginary i*/
eye.c=1.0;

for (i=1; i<=N; i++)          /* Initializes M matrices to zero */
  {
  for (j=1; j<=3; j++)
    {
    M[i][j].r=0.0; M[i][j].c=0.0;
    Ms[i][j].r=0.0; Ms[i][j].c=0.0;
    }                     /* End j loop */
  }                       /* End i loop */

for (i=1; i<=N; i++)
  {
  V[i].r=0.5*fabs((cos(2.0*i*dx)))-(e*F*i*dx);
  V[i].c=0.0;
  }
```

```
for (i=1; i<=N; i++)  /* This initializes the M matrices in sparse format */
  {
  if (i==1)
    {
    M[i][2].r=1.0;
    M[i][2].c=-1.0*(c1*V[i].r+2*c1*c2);
    Ms[i][2]=Cconj(M[i][2]);
    M[i][3].r=0.0;
    M[i][3].c=c1*c2;
    Ms[i][3]=Cconj(M[i][3]);
    }                      /* End if */
  else if (i==N)
    {
    M[N][1].r=0.0;
    M[N][1].c=c1*c2;
    Ms[N][1]=Cconj(M[N][1]);
    M[N][2].r=1.0;
    M[N][2].c=-1.0*(c1*V[i].r+2*c1*c2);
    Ms[N][2]=Cconj(M[N][2]);
    }                      /* End else if*/
  else
    {
    M[i][1].r=0.0;
    M[i][3].r=0.0;
    M[i][1].c=c1*c2;
    M[i][3].c=c1*c2;
    Ms[i][1]=Cconj(M[i][1]);
    Ms[i][3]=Cconj(M[i][3]);
    M[i][2].r=1.0;
    M[i][2].c=-1*(c1*V[i].r+2*c1*c2);
    Ms[i][2]=Cconj(M[i][2]);
    }                      /* End else */
  }                        /* End i loop*/


for (i=1; i<=N; i++)
  {
  psi[i].r=0.0;
  psi[i].c=0.0;
  }                        /* End i loop */
```

```c
for (i=1; i<=N; i++)
  {
  psi[i].r=0.6*exp(-1*(i-5001.0)*(i-5001.0)/(2*sigma));
  psi[i].c=0.0;                    /* Remember - make divisor float */
  psit[i]=Ceq(psi[i]);
  }                                /* End for i */


for (j=1; j<=N; j++)
  {

  conj[j]=Cconj(psi[j]);
  magipsi[j]=Cmult(conj[j],psi[j]);
  }                                /* End j loop */




/*LU Decomp procedure */

for (i=1; i<=N; i++)
  {
  L[i][1].r=1.0;
  L[i][1].c=0.0;         /* Initializes Lower main diagonal */
  }                      /* End for i */

 U[1][1]=Ceq(Ms[1][2]);      /* Initializes first Upper value */

 L[1][2]=Cdiv(one,U[1][1]);      /* Initializes first lower value */
 L[1][2]=Cmult(L[1][2],Ms[2][1]);


for (j=1; j<=N; j++)
  {
  U[j][2]=Ceq(Ms[j][3]);   /* Solves next 2 Upper values */
  temp=Cmult(L[j][2],U[j][2]);
  U[j+1][1]=Csub(Ms[j+1][2],temp);


  L[j+1][2]=Cdiv(one,U[j+1][1]);   /* Calculates next Lower value */
  L[j+1][2]=Cmult(L[j+1][2],Ms[j+1][1]);
  }                                /* End j loop */
```

```
for (loop=0; loop<=16000; loop++)

{

for (i=1; i<=N; i++)
  {
    sum.r=0.0; sum.c=0.0;          /* This creates "b" vector */
     if (i==1)
       {
        temp=Cmult(M[i][2],psit[1]);
        sum=Cadd(sum,temp);
        temp1=Cmult(M[i][3],psit[2]);
        sum=Cadd(sum,temp1);
       }                    /* End if */
     else if (i==N)
       {
        temp=Cmult(M[i][1],psit[N-1]);
        sum=Cadd(sum,temp);
        temp1=Cmult(M[i][2],psit[N]);
        sum=Cadd(sum,temp1);
       }                        /* End else if */
     else
       {
        for (j=1; j<=3; j++)
          {
           temp=Cmult(M[i][j],psit[(i-1)+(j-1)]);
           sum=Cadd(sum,temp);
          }                         /* End j */
       }                    /* End  else */
      b[i]=Ceq(sum);
   }                        /* End i */



y[1]=Cdiv(b[1],L[1][1]);

for (i=2;i<=N; i++)
  {
    sum.r=0.0; sum.c=0.0;


    temp=Cmult(L[i-1][2],y[i-1]); /* Solves intermediate matrix */
    sum=Csub(b[i],temp);
```

```c
      temp=Cdiv(one,L[i][1]);
      y[i]=Cmult(temp,sum);
      }                          /* End i loop */


  npsi[N]=Cdiv(y[N],U[N][1]);

  for (i=N-1;i>=1;i--)
     {
     sum.r=0.0; sum.c=0.0;

     temp=Cmult(U[i][2],npsi[i+1]);  /* Solves final answer */
     sum=Csub(y[i],temp);

     temp=Cdiv(one,U[i][1]);
     npsi[i]=Cmult(temp,sum);
     }                          /* End i loop */


  for (j=1; j<=N; j++)
     {

     nconj[j]=Cconj(npsi[j]);
     nmagpsi[j]=Cmult(nconj[j],npsi[j]);
     }                          /* End j loop */


  if (loop%100==0)
     {
        for (j=1; j<=N; j++)
          {
          printf("%.3f ",nmagpsi[j].r);
          }
        printf(" \n");

     }



  for (j=1; j<=N; j++)
     {
     psit[j]=Ceq(npsi[j]);
     }                          /* End j loop */
```

```
}                    /* End loop loop */


return;

}              /* End program */

struct complex Cadd (struct complex x, struct complex y)


{
struct complex z;


z.c=x.c+y.c;
z.r=x.r+y.r;
return z;
}

struct complex Csub (struct complex x, struct complex y)


{
struct complex z;


z.c=x.c-y.c;
z.r=x.r-y.r;
return z;
}

struct complex Cmult (struct complex x, struct complex y)


{
struct complex z;


z.c=x.r*y.c + y.r*x.c;
z.r=x.r*y.r - x.c*y.c;

return z;
}

struct complex Cdiv (struct complex x, struct complex y)


{
struct complex z;
double d;
```

45

```
d=(1.0/((y.r*y.r)+(y.c*y.c)));
z.r=d*((x.r*y.r)+(x.c*y.c));
z.c=d*((x.c*y.r)-(x.r*y.c));

return z;
}

struct complex Ceq (struct complex x)

{
struct complex z;

z.r=x.r;
z.c=x.c;

return z;

}

struct complex Cconj(struct complex x)

{
struct complex z;

z.r=x.r;
z.c=-1.0*x.c;

return z;
}
```

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